Mathematical Determination of Breath
## Alcohol Concentration
In the BAC Verifier Datamaster

The BAC Verifier Datamaster employs an algorithm derived from Beer's Law to compute the breath alcohol concentration (BrAC). Beer's Law relates the decrease in radiant energy transmittance to the increase in concentration of the energy absorbing analyte (ethanol). As the concentration of analyte increases, the transmittance of energy through the sample cell decreases in an exponential fashion. Beer's law further assumes monochromatic light, closely approximated by the filters in the instrument. Beer's Law is described with the following differential equation:

$$\frac{dI}{dC} = -kI \qquad\qquad Eq.\ 1$$

Equation 1 is viewed graphically as:
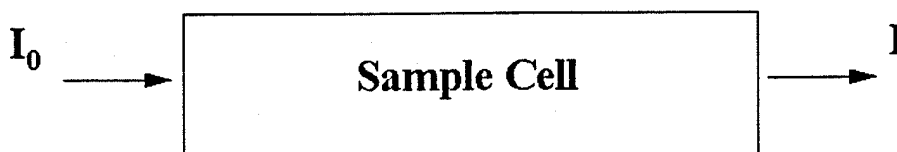
$$I_0 \longrightarrow \boxed{\textbf{Sample Cell}} \longrightarrow I$$

The decrease in transmitted light (I) is a function of analyte concentration (C) with the fractional decrease (dI) being constant throughout the sample cell. The solution to Equation 1 is:

$$T = \frac{I}{I_0} = e^{-abc} \qquad\qquad Eq.\ 2$$

where: T = transmittance
a = the molar absorptive constant for ethanol at the particular wavelength used in the BAC Datamaster
b = pathlength
c = concentration of analyte (ethanol)

The absorbance (A) of light energy can be derived from the transmittance in Equation 2 according to:

$$A = -\ln T = -\ln \frac{I}{I_0} = abc \qquad Eq.\ 3$$

The values of a and b in Equation 3 can be combined to form the value k and restated as:

$$-\ln \frac{I}{I_0} = kc \qquad Eq.\ 4$$

Since the BAC Datamaster is designed to measure the concentration of ethanol in the sample chamber, we are interested in solving Equation 4 for C according to:

$$c = -\frac{1}{k} \ln \frac{I}{I_0} \qquad Eq.\ 5$$

The instrument now determines the concentration of ethanol by measuring a final processed DC voltage at test point 6 on the detector board. As the concentration of alcohol increases and the transmittance of radiant light to the detector decreases, the voltage at TP6 increases. The voltage (V) will thus be proportional to some circuit gain (Z) times the change (decrease) in radiant light. Next, we must express I/I_0 of Equation 5 in terms of the voltage (V). This is accomplished as follows:

$$V = Z(I_0 - I)$$

where: Z = circuit gain

The next several steps will determine an equation where I/I_0 is expressed in terms of V:

$$V = ZI_0 - ZI$$

$$0 = ZI_0 - ZI - V$$

$$0 = \frac{ZI_0 - ZI - V}{ZI_0}$$

$$0 = \frac{ZI_0}{ZI_0} - \frac{ZI}{ZI_0} - \frac{V}{ZI_0}$$

$$0 = 1 - \frac{I}{I_0} - \frac{V}{ZI_0}$$

$$\frac{I}{I_0} = 1 - \frac{V}{ZI_0} \qquad\qquad Eq.\ 6$$

Equation 6 now expresses I/I_0 in terms of V allowing us to substitute this expression back into Equation 5 and obtain:

$$c = -\frac{1}{k} \ln\left[1 - \frac{V}{ZI_0}\right] \qquad\qquad Eq.\ 7$$

As noted above the constant 1/k is empirically determined based on the pathlength employed in the Datamaster and the molar absorptive properties of ethanol at the wavelength employed (3.44μ). The value of 1/k has been set equal to 1.27665. Expressing 1/k to five digits of precision is really unnecessary since the instrument effectively recomputes it with each measurement as discussed below. The value of ZI_0 is also a constant in Equation 7 which must always be greater than the maximum voltage V. The value of ZI_0 has been set equal to 5.

Equation 7 can now be simplified to:

$$C = X_a = k_1 [\ln(1 - \frac{V}{k_2})]$$ *Eq.* 8

where: X_a is the expression for C in the software code

Incorporating the constants into Equation 8 we obtain:

$$X_a = -1.27665 [\ln(1 - \frac{V}{5})]$$ *Eq.* 9

Application of Taylor's Approximating Polynomial

The Taylor's series polynomial is an approximating function used in computations where a direct analytical result may not be possible. When computing the breath alcohol concentration (BrAC) the BAC Datamaster needs to perform a natural logarithmic (ln) calculation which is unavailable in the instruction set for the microprocessor. As a result, an approximating function not requiring the natural log function is employed. This is where Taylor's approximating polynomial is applied.

The function within the Datamaster that needs to be computed to determine breath alcohol concentration is:

$$X_a = k_1 [\ln(1 - \frac{V}{k_2})]$$ *Eq.* 10

where: X_a = the computed BrAC
k_1 = a constant derived from the Beer-Lambert
law incorporating the path length
and molar absorptive constant for
ethanol
V = the DC voltage from the detector board
that is proportional to BrAC
k_2 = a constant chosen to ensure that V/k_2
is never greater than 1

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The appropriate values for k_1 and k_2 have been determined for the Datamaster instrument and when incorporated into Equation 10 yield:

$$X_a = -1.27665\left[\ln\left(1 - \frac{V}{5}\right)\right] \qquad Eq.\ 11$$

The maximum output of the analog-to-digital converter is 1.999 VDC which represents the maximum value of V. Thus, $k_2=5$ is adequate to ensure $V/k_2 < 1$.

Taylor's approximating polynomial has the following general form:

$$f(x) = \sum_{k=0}^{n} \frac{(x-a)^k\, f^k(a)}{k!} \qquad Eq.\ 12$$

where: a = the value of x around which we are approximating f(x)

f^k = the kth derivative of the function f evaluated at a

Expanding Equation 12 we obtain:

$$f(x) = f(a) + (x-a)\, f^1(a) + \frac{(x-a)^2}{2!} f^2(a) + \cdots + \frac{(x-a)^n}{n!} f^n(a) \qquad Eq.\ 13$$

Taylor's expansion can only be applied to functions that are continuously differentiable at x=a, which is the case in ln(1-x). In the Datamaster, Taylor's approximation needs to be expanded about a=0 since this will eliminate the ln function from the approximation. This means that Taylor's approximation will be most accurate at or near zero. Inaccuracy increases as we depart from zero. However, including enough terms in the polynomial will ensure sufficient accuracy within the relevant range.

The Datamaster employs the first four terms of Taylor's approximation seen in Equation 13. If we let a=0 and expand Taylor's polynomial about a=0 and include the first four terms we obtain:

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$$f(x) = f(0) + (x-0)f^1(0) + \frac{(x-0)^2}{2}f^2(0) + \frac{(x-0)^3}{6}f^3(0) \qquad Eq. \ 14$$

The following are the derivatives of $f(x) = \ln(1-x)$ where $x = v/5$. These derivatives are evaluated at $x=0$:

$$f(x) = \ln(1 - x)$$

$$f^1(x) = -(1 - x)^{-1} \ \Rightarrow \ f^1(0) = -1$$

$$f^2(x) = -(1 - x)^{-2} \ \Rightarrow \ f^2(0) = -1$$

$$f^3(x) = -2(1 - x)^{-3} \ \Rightarrow \ f^3(0) = -2$$

One could also perform the expansion by choosing $x=v/5$ to be negative. In this case we would be expanding $\ln(1+x)$ and arrive at an alternating series. The results are the same either way. Incorporating the derivatives above into Equation 14 we obtain:

$$f(x) = 0 - x - \frac{x^2}{2} - \frac{x^3}{3} \qquad Eq. \ 15$$

To obtain f(x) in terms of BrAC we need to incorporate the k_1 constant as follows:

$$f(x) = -1.27665\left(- x - \frac{x^2}{2} - \frac{x^3}{3}\right) \qquad Eq. \ 16$$

where: $x = v/5$

Since Taylor's expansion is approximating another function [$\ln(1-x)$] about the point $x=a$ (here $a=0$) the accuracy will decrease as one departs further from a. Because the application of Taylor's expansion involves a finite number of terms (three in the Datamaster) there will be an error due to truncation. A

convenient way to approximate this error or find an upper bound for it is available. Consider Taylor's expansion expressed as:

$$f(x) = P_k(x) + R_k(x)$$

where: $P_k(x)$ = the polynomial expanded to k terms
$R_k(x)$ = the remainder term

The remainder term $R_k(x)$ is the error resulting from using only k terms in the approximation. $R_k(x)$ is simply the $k+1^{st}$ term in the expansion as follows:

$$f(x) = f(a) + (x-a) \, f^1(a) + \cdots + \frac{(x-a)^{k+1}}{(k+1)!} f^{k+1}(c) \qquad Eq. \ 17$$

where: c = a value lying between a and x. Select
c to be equal to the greater of the two
in order to maximize the error estimate
f^k = the kth derivative of f(x)

The last term in Equation 17 is the error term due to truncating the series to k terms. This is expressed as:

$$|R_n(x)| = \left| \frac{(x-a)^{k+1}}{(k+1)!} f^{k+1}(c) \right| \qquad Eq. \ 18$$

Letting a=0, k=4, and c=0.08 (to maximize the error estimate) we obtain:

$$|R_n(0.08)| = -1.27665 \left| \frac{(x)^4}{(4)!} f^4(0.08) \right| < 0.0000184 \qquad Eq. \ 19$$

where: x = 0.08 results from V = 0.4 VCD on the
detector board corresponding to an
approximate BrAC of 0.106 g/210L

Equation 19 reveals the maximum error resulting from using four terms in Taylor's expansion at a BrAC level of approximately 0.106 g/210L. This is equivalent to fourth decimal place accuracy (0.5×10^{-4}) and is below the resolution of the analog-to-digital converter employed in the Datamaster (± 1.0 mV DC corresponding approximately to 0.000255 g/210L). Employing the

three terms (to the third derivative) is clearly more than adequate.

Similar to above we can evaluate the error associated with employing only two terms (to the second derivative) in Taylor's expansion near the 0.100 g/210L level. Again, consider the remainder function in Equation 18 above. We now determine its magnitude employing only to the third term (remembering that the first term is zero):

$$|R_n(0.08)| = -1.27665 \left| \frac{(x)^3}{(3)!} f^3(0.08) \right| < 0.000280 \qquad Eq. \ 20$$

Equation 20 reveals an error of 0.000280 g/210L at 0.106 g/210L when using only two terms. Clearly, this would be adequate even for forensic purposes at the critical per se level of 0.100 g/210L.

Another important point to be made is that Taylor's expansion as employed in the Datamaster is always less than the direct analytical result. As concentration increases and the error in Taylor's expansion increases, the approximated value is even lower than the direct analytical result. A comparison of the direct analytical result and Taylor's approximation at four different concentrations are shown below:

Concentration	Analytical Result	Taylor's Approximation	Difference
0.01	0.0128	0.0128	3.2×10^{-9}
0.10	0.106449	0.106435	0.000014
0.20	0.20748	0.207296	0.000184
0.30	0.300935	0.300188	0.000747

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The figure below illustrates the BrAC computed by both the direct
analytical approach and Taylor's approximation and plotted
against the final processed DC voltage at the detector board.
Their differences are not apparent until higher alcohol
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ns.

**Both The Analytical and Taylor's Approximation
As a Function of Instrument Voltage**

BrAC (g/210L)
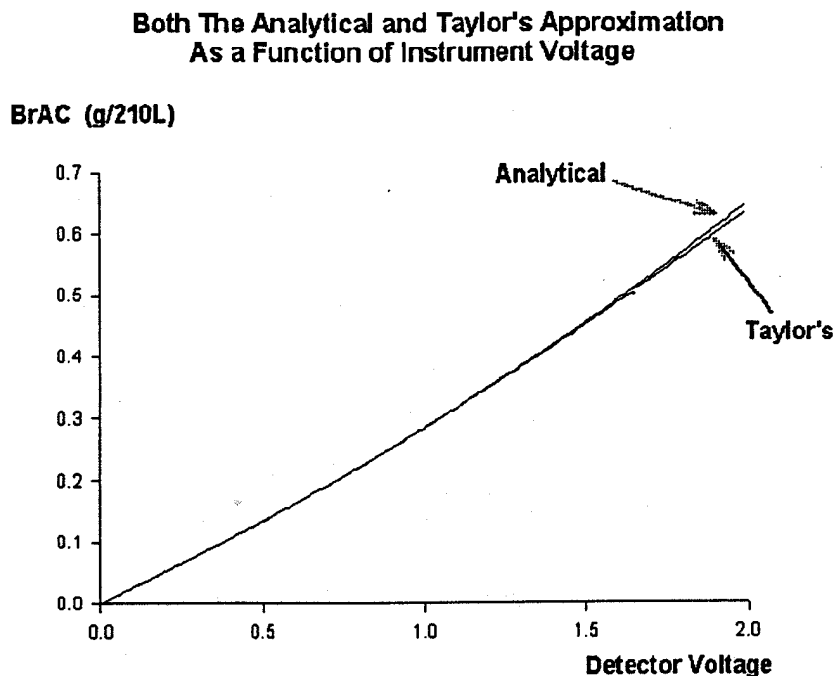
Taylor's approximating polynomial is clearly being appropriately
applied in the BAC Datamaster.

Final Computations

        We next consider how the BAC Datamaster determines the final
breath alcohol concentration result. As discussed above, the
instrument incorporates the DC voltage on the detector board
(TP6) into the following equation:

$$X_a = -1.27665 \left[\ln\left(1-\frac{V}{5}\right)\right] = -1.27665\left[-\frac{V}{5} - \frac{(\frac{V}{5})^2}{2} - \frac{(\frac{V}{5})^3}{3}\right] \qquad Eq.\ 21$$

where: X_a = ethanol concentration at the 3.44μm
            filter
        X_{ac} = the ethanol concentration at the 3.37μm
            filter which is substituted for X_a when
            that filter is in place

The instrument next removes the absorbance at each filter by subtracting the absorbance due to water:

$$X_a - b_1 = X_a'$$

where: b_1 = water absorbance at 3.44μm
        b_2 = water absorbance at 3.37μm

Next, the instrument corrects for a calibration value (CAL) and the internal standard (quartz plate) value according to:

$$X_a'' = CAL \cdot X_Q \cdot X_a' \qquad\qquad Eq.\ 22$$

where:

$$CAL = \frac{C_{ap}}{X_{acal}} \qquad\qquad X_Q = \frac{X_{Qcal}}{X_{Qtst}}$$

where: C_{ap} = the value of the calibration solution as
            determined by the state toxicology
            reference lab
        X_{acal} = the value measured by the instrument at
            the time of calibration

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X_{Qcal} = the value of the quartz plate at the time of calibration

X_{Qtst} = the value of the quartz plate at the time of the field analysis

Equation 22 illustrates the diminished value of the constant (1.27665) in Equation 9. The value of CAL and the changing value of X_Q continually adjust the constant for a specific analysis that is consistent with the optics, electronics, etc. at the time of analysis. Moreover, the validity of these constants are determined by analysis of the external simulator standard at the time of each subject test.

Finally, the instrument determines the presence of an interfering substance (acetone) according to the following:

$$C_a = (A \cdot X''_{ac}) - (B \cdot X''_a) \qquad\qquad Eq.\ 23$$

where: C_a = a computed ethanol value
A,B = constants determined during calibration based on absorbance of ethanol and acetone

Next, the value of $X''_a - C_a$ is determined. If this exceeds the threshold set in the instrument (0.01) then C_a becomes the reported ethanol result and the difference becomes the reported "Interferant" result. If the difference does not exceed the threshold, then X''_a becomes the reported ethanol result or breath alcohol concentration.

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